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Reciprocal complementary Wiener numbers of trees, unicyclic graphs and bicyclic graphs

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ABSTRACT

The reciprocal complementary Wiener number of a connected graph G is defined as

$$\mathrm{RCW}(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d + 1 - d(u, v|G)}$$

where $V(G)$ is the vertex set, $d(u, v|G)$ is the distance between vertices u and v, d is the diameter of G. We determine the trees with the smallest, the second smallest and the third smallest reciprocal complementary Wiener numbers, and the unicyclic and bicyclic graphs with the smallest and the second smallest reciprocal complementary Wiener numbers.

1. Introduction

Numbers reflecting certain structural features of a molecule that are derived from its molecular graph are known as topological indices. The Wiener number (often also called the Wiener index) is one of the oldest such topological indices [20,1,7,19] and it has been studied extensively [5,6]. It found applications in structure–property and structure–activity models, and in the computational screening of chemical libraries for biologically active compounds — see, e.g., [16,2]. Its mathematical properties may be found in [3,4] and it is still a topic of current research, e.g., [17,21,22].

Since the Wiener number was formalized via the distance matrix [8], various Wiener-like molecular descriptors have been proposed — see, e.g., [18]. For recent reviews of matrices and topological indices related to the Wiener index, see [9,10,15]. The reciprocal complementary Wiener (RCW) number is one of the newest additions in the family of such descriptors. It was put forward by Ivanciuc [11] and its (chemical) applications were discussed in [11–14].

Let G be a simple connected graph with vertex set $V(G)$. For vertices $u, v \in V(G)$, $d(u, v|G)$ denotes the distance between u and v in G. Then the RCW number of G is defined as [11]

$$\mathrm{RCW}(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d + 1 - d(u, v|G)}$$

where d is the diameter, and the summation goes over all unordered pairs of distinct vertices of G. Some properties, especially various upper and lower bounds for the RCW number and Nordhaus–Gaddum-type result, have been obtained in [23].

Recall that a connected graph with n vertices is known as a tree, a unicyclic graph and a bicyclic graph if it possesses $n - 1$, n and $n + 1$ edges, respectively. In [23], the largest RCW number for graphs with given numbers of vertices and edges

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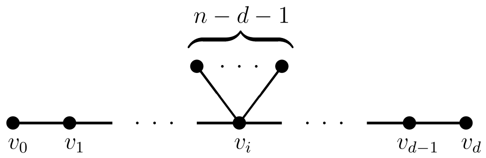

Fig. 1. The tree $P_{n,d,i}$.

has been determined. In continuation of the study on the RCW number, we establish further properties of the RCW number. In particular, we determine the trees with the smallest, the second smallest and the third smallest RCW numbers, and the unicyclic and bicyclic graphs with the smallest and the second smallest RCW numbers.

2. RCW numbers of trees

Let P_n be the n-vertex path. Recall that a caterpillar is a tree in which removal of all pendent vertices (i.e., those of degree one) gives a path. Let $P_{n,d,i}$ be the tree formed from the path P_{d+1} whose vertices are labelled consecutively as $v_0, v_1, \ldots, v_d$ by attaching $n-d-1$ pendent vertices to vertex v_i, where $1 \le i \le d-1$ and $2 \le d \le n-2$ (see Fig. 1). Since $P_{n,d,i} = P_{n,d,d-i}$, we may require $1 \le i \le \lfloor \frac{d}{2} \rfloor$. Let $\mathbb{T}(n, d)$ be the class of trees with n vertex and diameter d, where $3 \le d \le n-2$.

For a tree T and $v \in V(T)$, the component of $T - v$ containing the neighbor u of v in T is called the branch of T at u, whose vertex set is denoted by $B_v(u)$.

Lemma 1. *Let $T \in \mathbb{T}(n, d)$, where $3 \le d \le n-2$. If T is not a caterpillar, then there is a caterpillar T^* such that* $\mathrm{RCW}(T) > \mathrm{RCW}(T^*)$.

Proof. Let $P(T) = v_0v_1 \ldots v_d$ be a diameter-achieving path of T. Since T is not a caterpillar, it follows that for some i with $2 \le i \le d-2$, v_i has a non-pendent neighbor w outside $P(T)$. Let $V_1 = B_{v_i}(w) - \{w\}$ and $V_2 = V(T) - B_{v_i}(w)$.

Let T' denote the tree formed from T by deleting edges wu and adding edges v_iu for all neighbors u of w different from v_i. Obviously $T' \in \mathbb{T}(n, d)$.

For $u \in V_1$ and $v \in V_2$, $d(u, v|T') = d(u, v|T) - 1$ and then

$$\frac{1}{d+1-d(u,v|T)} > \frac{1}{d+1-d(u,v|T')}.$$

Note that $h(x) = \frac{1}{d+1-(x+1)} - \frac{1}{d+1-x}$ is increasing for $1 \le x \le d-1$. For $u \in V_1$, we have $d(u, v_d|T') = d(u, v_d|T) - 1$, $d(u, w|T') = d(u, w|T) + 1$, $d(u, v_d|T') > d(u, w|T)$, and then

$$\begin{aligned}&\frac{1}{d+1-d(u,v_d|T)} - \frac{1}{d+1-d(u,v_d|T')} - \left(\frac{1}{d+1-d(u,w|T')} - \frac{1}{d+1-d(u,w|T)}\right)\\ &\quad = h\left(d(u,v_d|T')\right) - h\left(d(u,w|T)\right) > 0.\end{aligned}$$

It follows that

$$\begin{aligned}\mathrm{RCW}(T) - \mathrm{RCW}(T') &= \sum_{u\in V_1}\sum_{v\in V_2}\frac{1}{d+1-d(u,v|T)} - \sum_{u\in V_1}\sum_{v\in V_2}\frac{1}{d+1-d(u,v|T')}\\ &\quad + \sum_{u\in V_1}\frac{1}{d+1-d(u,w|T)} - \sum_{u\in V_1}\frac{1}{d+1-d(u,w|T')}\\ &> \sum_{u\in V_1}\left(\frac{1}{d+1-d(u,v_d|T)} - \frac{1}{d+1-d(u,v_d|T')}\right)\\ &\quad - \sum_{u\in V_1}\left(\frac{1}{d+1-d(u,w|T')} - \frac{1}{d+1-d(u,w|T)}\right)\\ &= \sum_{u\in V_1}\left(h\left(d(u,v_d|T')\right) - h\left(d(u,w|T)\right)\right) > 0\end{aligned}$$

and then $\mathrm{RCW}(T) > \mathrm{RCW}(T')$. Iterating the transformation from T to T' will finally yield the tree T^* as required. $\square$

Let $\widehat{V}(T)$ be the set of vertices in a tree T with degree at least three.

Lemma 2. *Let $T \in \mathbb{T}(n, d)$ be a caterpillar. If $|\widehat{V}(T)| \ge 2$, then there is an i with $1 \le i \le d-1$ such that* $\mathrm{RCW}(T) > \mathrm{RCW}(P_{n,d,i})$.

Proof. Let $P = v_0 v_1 \ldots v_d$ be a diameter-achieving path of T. Let N_i be the set of neighbors of v_i outside the path P for $1 \le i \le d-1$.

First suppose that there are vertices $v_k, v_j \in \widehat{V}(T)$ such that $k < j \le \lfloor \frac{d}{2} \rfloor$ (if there are vertices $v_k, v_j \in \widehat{V}(T)$ such that $\lfloor \frac{d}{2} \rfloor \ge j > k$, the proof is similar). Choose the smallest such integers k and j. Let $W = V(T) - N_k - V(P)$. Let T' denote the tree formed from T by deleting edges $v_k u$ and adding edges $v_j u$ for all $u \in N_k$. Obviously $T' \in \mathbb{T}(n, d)$.

For $u \in N_k$ and $v \in W$, we have $d(u, v|T') < d(u, v|T)$ and then

$$\frac{1}{d+1-d(u,v|T)} > \frac{1}{d+1-d(u,v|T')}.$$

For $u \in N_k$, the $d+1$ distances between u and vertices in $P(T)$ (resp. $P(T')$) are $1, 2, 2, 3, 3, \ldots, k+1, k+1, k+2, k+3, \ldots, d-k+1$ (resp. $1, 2, 2, 3, 3, \ldots, j+1, j+1, j+2, j+3, \ldots, d-j+1$). For $u \in N_k$, comparing these distances in T and T' and bearing in mind $k < j \le \lfloor \frac{d}{2} \rfloor$, we have

$$\sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T)} > \sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T')}.$$

Now for $u \in N_k$, we have

$$\begin{aligned}
\mathrm{RCW}(T) - \mathrm{RCW}(T') &= |N_k| \left(\sum_{v \in W} \frac{1}{d+1-d(u,v|T)} - \sum_{v \in W} \frac{1}{d+1-d(u,v|T')} \right) \\
&\quad + |N_k| \left(\sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T)} - \sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T')} \right) \\
&> 0
\end{aligned}$$

and then $\mathrm{RCW}(T) > \mathrm{RCW}(T')$. Iterating the transformation from T to T' will yield a tree T_1 such that $\mathrm{RCW}(T) > \mathrm{RCW}(T_1)$, $|\widehat{V}(T_1)| \le 2$ and if $\widehat{V}(T_1) = \{v_{k_1}, v_{j_1}\}$ then $k_1 \le \lfloor \frac{d}{2} \rfloor \le \lceil \frac{d}{2} \rceil \le j_1$.

Now suppose that $|\widehat{V}(T)| = 2$ and $\widehat{V}(T) = \{v_k, v_j\}$ such that $k \le \lfloor \frac{d}{2} \rfloor \le \lceil \frac{d}{2} \rceil \le j$. Assume that $\lfloor \frac{d}{2} \rfloor - k \le j - \lceil \frac{d}{2} \rceil$. By deleting edges $v_j u$ and adding edges $v_k u$ for all $u \in N_j$ we get the tree $P_{n,d,k}$. Let $T' = P_{n,d,k}$.

Note that for $u \in N_j$ and $v \in N_k$,

$$\frac{1}{d+1-d(u,v|T)} > \frac{1}{d+1-d(u,v|T')},$$

and by similar arguments as above, for $u \in N_j$, we have

$$\sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T)} > \sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T')}.$$

Then for $u \in N_j$, we have

$$\begin{aligned}
\mathrm{RCW}(T) - \mathrm{RCW}\left(P_{n,d,k}\right) &= |N_j| \left(\sum_{v \in N_k} \frac{1}{d+1-d(u,v|T)} - \sum_{v \in N_k} \frac{1}{d+1-d(u,v|T')} \right) \\
&\quad + |N_j| \left(\sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T)} - \sum_{v \in V(P)} \frac{1}{d+1-d(u,v|T')} \right) \\
&> 0
\end{aligned}$$

and then $\mathrm{RCW}(T) > \mathrm{RCW}\left(P_{n,d,k}\right)$. This proves the lemma. $\square$

Lemma 3. *For $P_{n,d,i}$ with $4 \le d \le n-2$, $1 \le i \le d-1$ and $i \ne \lfloor \frac{d}{2} \rfloor, \lceil \frac{d}{2} \rceil$, we have*

$$\mathrm{RCW}\left(P_{n,d,i}\right) > \mathrm{RCW}\left(P_{n,d,\lfloor \frac{d}{2} \rfloor}\right).$$

Proof. Suppose, without loss of generality, that $1 \le i < \lfloor \frac{d}{2} \rfloor$. Let $T_1 = P_{n,d,i}$ and $T_2 = P_{n,d,\lfloor \frac{d}{2} \rfloor}$. By similar arguments as above, for any vertex u of the $n-d-1$ vertices outside the path $v_0 v_1 \ldots v_d$, we have

$$\sum_{i=0}^{d} \frac{1}{d+1-d(u,v_i|T_1)} > \sum_{i=0}^{d} \frac{1}{d+1-d(u,v_i|T_2)}$$

and then,

$$\mathrm{RCW}\left(P_{n,d,i}\right) - \mathrm{RCW}\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right) = (n-d-1)\left(\sum_{i=0}^{d}\frac{1}{d+1-d(u,v_i|T_1)} - \sum_{i=0}^{d}\frac{1}{d+1-d(u,v_i|T_2)}\right) > 0.$$

Now the result follows. □

Theorem 1. *Let $T \in \mathbb{T}(n,d)$ and $T \neq P_{n,d,\lfloor\frac{d}{2}\rfloor}$, where $3 \leq d \leq n-2$. Then $\mathrm{RCW}(T) > \mathrm{RCW}\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right)$.*

Proof. If T is not a caterpillar, then we have by Lemma 1 that there is a caterpillar $T' \in \mathbb{T}(n,d)$ such that $\mathrm{RCW}(T) > \mathrm{RCW}(T')$. If T is a caterpillar with $|\widehat{V}(T)| \geq 2$, then we have by Lemma 2 that for some i with $1 \leq i \leq d-1$, $\mathrm{RCW}(T) > \mathrm{RCW}(P_{n,d,i})$. Now the result follows from Lemma 3. □

Lemma 4. *For $2 \leq d \leq n-2$, $\mathrm{RCW}\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right) > \mathrm{RCW}\left(P_{n,d+1,\lfloor\frac{d+1}{2}\rfloor}\right)$, where $P_{n,n-1,\lfloor\frac{n-1}{2}\rfloor} = P_n$.*

Proof. Let $x = 0$ for even d and 1 for odd d. Then

$$\mathrm{RCW}\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right) = d + (n-d-1)\left(\frac{n-d-2}{2(d-1)} + \sum_{j=1}^{\lfloor\frac{d}{2}\rfloor}\frac{2}{d-j} + \frac{1}{d} + \frac{2x}{d-1}\right).$$

If d is even, then

$$\begin{aligned}
\mathrm{RCW}\left(P_{n,d,\frac{d}{2}}\right) - \mathrm{RCW}\left(P_{n,d+1,\frac{d}{2}}\right) &= -1 + (n-d-1)\left(\frac{n-d-2}{2(d-1)} + \sum_{j=1}^{\frac{d}{2}}\frac{2}{d-j} + \frac{1}{d}\right) \\
&\quad - (n-d-2)\left(\frac{n-d-3}{2d} + \sum_{j=0}^{\frac{d}{2}-1}\frac{2}{d-j} + \frac{1}{d+1} + \frac{2}{d}\right) \\
&> -1 + (n-d-1)\left(\sum_{j=0}^{\frac{d}{2}}\frac{2}{d-j} - \frac{1}{d}\right) - (n-d-2)\left(\sum_{j=0}^{\frac{d}{2}}\frac{2}{d-j} - \frac{2}{d} + \frac{1}{d+1}\right) \\
&= -1 + \sum_{j=0}^{\frac{d}{2}}\frac{2}{d-j} + \frac{n-d-3}{d} - \frac{n-d-2}{d+1} \\
&> -1 + \sum_{j=0}^{\frac{d}{2}-1}\frac{2}{d} = 0.
\end{aligned}$$

If d is odd, then

$$\begin{aligned}
&\mathrm{RCW}\left(P_{n,d,\frac{d-1}{2}}\right) - \mathrm{RCW}\left(P_{n,d+1,\frac{d+1}{2}}\right) \\
&= -1 + (n-d-1)\left(\frac{n-d-2}{2(d-1)} + \sum_{j=1}^{\frac{d-1}{2}}\frac{2}{d-j} + \frac{1}{d} + \frac{2}{d-1}\right) - (n-d-2)\left(\frac{n-d-3}{2d} + \sum_{j=0}^{\frac{d-1}{2}}\frac{2}{d-j} + \frac{1}{d+1}\right) \\
&> -1 + (n-d-1)\left(\sum_{j=0}^{\frac{d-1}{2}}\frac{2}{d-j} - \frac{1}{d} + \frac{2}{d-1}\right) - (n-d-2)\left(\sum_{j=0}^{\frac{d-1}{2}}\frac{2}{d-j} + \frac{1}{d+1}\right) \\
&= -1 + \sum_{j=0}^{\frac{d-1}{2}}\frac{2}{d-j} + (n-d-1)\left(\frac{2}{d-1} - \frac{1}{d}\right) - \frac{n-d-2}{d+1} \\
&> -1 + \sum_{j=0}^{\frac{d-1}{2}}\frac{2}{d} > 0. \quad \square
\end{aligned}$$

In [23], we have shown that for any tree T with n vertices different from the path P_n, $\mathrm{RCW}(T) > \mathrm{RCW}(P_n) = n-1$. Now we have:

Theorem 2. *For $n \geq 7$,*

$$\mathrm{RCW}\,(P_n) < \mathrm{RCW}\left(P_{n,n-2,\lfloor \frac{n-2}{2} \rfloor}\right) < \mathrm{RCW}\left(P_{n,n-2,\lfloor \frac{n-4}{2} \rfloor}\right)$$

and $\mathrm{RCW}(T) > \mathrm{RCW}\left(P_{n,n-2,\lfloor \frac{n-4}{2} \rfloor}\right)$ *for any n-vertex tree T different from P_n, $P_{n,n-2,\lfloor \frac{n-2}{2} \rfloor}$ and $P_{n,n-2,\lfloor \frac{n-4}{2} \rfloor}$.*

Proof. Let T be a tree with n vertices and diameter d. Then $2 \leq d \leq n-1$. If $d = n-1$, then $T = P_n$. Suppose that $d = n-2$, then T is a tree $P_{n,n-2,i}$, where $1 \leq i \leq \lfloor \frac{n-2}{2} \rfloor$. We have

$$\mathrm{RCW}(P_{n,n-2,i}) = n - 2 + \sum_{k=2}^{i+2} \frac{1}{n-k} + \sum_{k=3}^{n-i} \frac{1}{n-k},$$

and thus $\mathrm{RCW}(P_{n,n-2,i})$ is monotonically decreasing for $1 \leq i \leq \lfloor \frac{n-2}{2} \rfloor$, which, together with Lemma 4, implies that

$$\begin{aligned}\mathrm{RCW}\,(P_n) &< \mathrm{RCW}\left(P_{n,n-2,\lfloor \frac{n-2}{2} \rfloor}\right)\\ &< \mathrm{RCW}\left(P_{n,n-2,\lfloor \frac{n-4}{2} \rfloor}\right) < \cdots < \mathrm{RCW}\left(P_{n,n-2,1}\right).\end{aligned}$$

Now suppose that $d \leq n-3$, by Theorem 1 and Lemma 4, we have $\mathrm{RCW}(T) \geq \mathrm{RCW}\left(P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}\right)$ with equality if and only if $T \cong P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}$. We need only show

$$\mathrm{RCW}\left(P_{n,n-2,\lfloor \frac{n-4}{2} \rfloor}\right) < \mathrm{RCW}\left(P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}\right).$$

Case 1. n is odd. Let $i = \lfloor \frac{n-4}{2} \rfloor = \frac{n-5}{2}$. Then for $n \geq 9$

$$\begin{aligned}&\mathrm{RCW}\left(P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}\right) - \mathrm{RCW}\left(P_{n,n-2,i}\right)\\
&= -1 + \frac{1}{n-4} + \sum_{k=4}^{\frac{n+3}{2}} \frac{4}{n-k} + \frac{2}{n-3} - \left(\sum_{k=2}^{i+2} \frac{1}{n-k} + \sum_{k=3}^{n-i} \frac{1}{n-k}\right)\\
&= \left(-1 + \sum_{k=4}^{\frac{n+3}{2}} \frac{2}{n-k}\right) + \frac{1}{n-4} + \sum_{k=3}^{\frac{n+3}{2}} \frac{2}{n-k} - \sum_{k=2}^{\frac{n-1}{2}} \frac{1}{n-k} - \sum_{k=3}^{\frac{n+5}{2}} \frac{1}{n-k}\\
&> 0 + \frac{1}{n-4} + \frac{2}{n-1} + \frac{2}{n-3} - \frac{1}{n-2} - \frac{2}{n-5}\\
&> \frac{2}{n-1} + \frac{1}{n-3} + \frac{1}{n-4} - \frac{2}{n-5}\\
&= \frac{2n^3 - 27n^2 + 108n - 131}{(n-1)(n-3)(n-4)(n-5)} > 0,\end{aligned}$$

and it is easily seen that $\mathrm{RCW}\left(P_{7,4,2}\right) - \mathrm{RCW}\left(P_{7,5,1}\right) = \frac{19}{30} > 0$.

Case 2. n is even. Let $i = \lfloor \frac{n-4}{2} \rfloor = \frac{n-4}{2}$. Then

$$\begin{aligned}&\mathrm{RCW}\left(P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}\right) - \mathrm{RCW}\left(P_{n,n-2,i}\right)\\
&= -1 + \frac{5}{n-4} + \sum_{k=4}^{\frac{n+2}{2}} \frac{4}{n-k} + \frac{2}{n-3} - \left(\sum_{k=2}^{i+2} \frac{1}{n-k} + \sum_{k=3}^{n-i} \frac{1}{n-k}\right)\\
&= \left(-1 + \sum_{k=4}^{\frac{n+2}{2}} \frac{2}{n-k}\right) + \frac{5}{n-4} + \sum_{k=3}^{\frac{n+2}{2}} \frac{2}{n-k} - \sum_{k=2}^{\frac{n}{2}} \frac{1}{n-k} - \sum_{k=3}^{\frac{n+4}{2}} \frac{1}{n-k}\\
&> 0 + \frac{5}{n-4} + \frac{2}{n-2} - \frac{1}{n-2} - \frac{2}{n-4}\\
&= \frac{1}{n-2} + \frac{3}{n-4} > 0.\end{aligned}$$

By combining Cases 1 and 2, the proof is completed. □

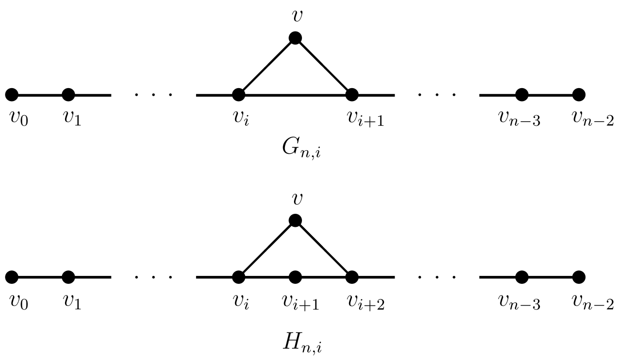

Fig. 2. The graphs $G_{n,i}$ and $H_{n,i}$.

By Theorem 2, P_n, $P_{n,n-2,\lfloor\frac{n-2}{2}\rfloor}$, $P_{n,n-2,\lfloor\frac{n-4}{2}\rfloor}$ are respectively the unique trees with the smallest, the second smallest and the third smallest RCW numbers in the class of trees with $n \ge 7$ vertices.

3. RCW numbers of unicyclic graphs

Let $G_{n,i}$ be the graph formed from the path P_{n-1} whose vertices are labelled consecutively as $v_0, v_1, \ldots, v_{n-2}$ by adding vertex v and edges vv_i, vv_{i+1}, where $0 \le i \le \lfloor\frac{n-3}{2}\rfloor$, and let $H_{n,i}$ be the graph formed from the path P_{n-1} by adding vertex v and edges vv_i, vv_{i+2} where $0 \le i \le \lfloor\frac{n-4}{2}\rfloor$ (see Fig. 2). For simplicity, we write G_i for $G_{n,i}$ and H_i for $H_{n,i}$.

Lemma 5. *The reciprocal complementary Wiener numbers of G_i for $0 \le i \le \lfloor\frac{n-3}{2}\rfloor$ and H_i for $0 \le i \le \lfloor\frac{n-4}{2}\rfloor$ are given by*

$$\mathrm{RCW}(G_i) = n - 2 + \sum_{k=2}^{i+2} \frac{1}{n-k} + \sum_{k=2}^{n-i-1} \frac{1}{n-k}$$

$$\mathrm{RCW}(H_i) = n - 2 + \sum_{k=2}^{i+2} \frac{1}{n-k} + \sum_{k=2}^{n-i-2} \frac{1}{n-k} + \frac{1}{n-3}.$$

Moreover, $\mathrm{RCW}(G_i)$ *(resp.* $\mathrm{RCW}(H_i)$*) is monotonically decreasing for $0 \le i \le \lfloor\frac{n-3}{2}\rfloor$ (resp. $0 \le i \le \lfloor\frac{n-4}{2}\rfloor$).*

Lemma 6 *([23]). Let G be a connected graph with n vertices and diameter $d \ge 1$. Then* $\mathrm{RCW}(G) \ge f(n, d)$*, where*

$$f(n, d) = d + 2(n - d - 1)\left(\frac{x}{d+1} + \sum_{i=0}^{\lfloor\frac{d}{2}\rfloor-1} \frac{1}{d-i}\right) + \frac{(n-d)(n-d-1)}{2d}$$

with $x = 0$ for even d and 1 for odd d. Moreover, $f(n, d) > f(n, d+1)$ for $1 \le d \le n-3$.

Lemma 7. *Let $n \ge 7$. If n is odd and $n < 12$, then*

$$\mathrm{RCW}\left(H_{\lfloor\frac{n-4}{2}\rfloor}\right) < \mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right) < \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right).$$

Otherwise,

$$\mathrm{RCW}\left(H_{\lfloor\frac{n-4}{2}\rfloor}\right) < \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right) < \mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right).$$

Proof. First suppose that n is odd. Then

$$\begin{aligned}
&\mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right) - \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right) \\
&= \sum_{k=2}^{\frac{n+1}{2}} \frac{1}{n-k} + \sum_{k=2}^{\frac{n+1}{2}} \frac{1}{n-k} - \left(\sum_{k=2}^{\frac{n-3}{2}} \frac{1}{n-k} + \sum_{k=2}^{\frac{n+3}{2}} \frac{1}{n-k} + \frac{1}{n-3}\right) \\
&= \frac{2}{n-1} + \frac{2}{n+1} - \frac{3}{n-3} = \frac{n^2 - 12n + 3}{(n-1)(n+1)(n+3)}.
\end{aligned}$$

Since $n^2 - 12n + 3 > 0$ if and only if $n > 12$, we have $\mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right) < \mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right)$ for $n > 12$.

If $n < 12$, then $\mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right) < \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right)$ and

$$\begin{aligned}
&\mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right) - \mathrm{RCW}\left(H_{\lfloor\frac{n-4}{2}\rfloor}\right)\\
&\quad= \sum_{k=2}^{\frac{n+1}{2}} \frac{1}{n-k} + \sum_{k=2}^{\frac{n+1}{2}} \frac{1}{n-k} - \left(\sum_{k=2}^{\frac{n-1}{2}} \frac{1}{n-k} + \sum_{k=2}^{\frac{n+1}{2}} \frac{1}{n-k} + \frac{1}{n-3}\right)\\
&\quad= \frac{n-5}{(n-1)(n-3)} > 0,
\end{aligned}$$

implying that $\mathrm{RCW}\left(H_{\lfloor\frac{n-4}{2}\rfloor}\right) < \mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right) < \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right)$.

Now suppose that n is even. Then

$$\begin{aligned}
\mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right) - \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right) &= \sum_{k=2}^{\frac{n}{2}} \frac{1}{n-k} + \sum_{k=2}^{\frac{n}{2}+1} \frac{1}{n-k} - \left(\sum_{k=2}^{\frac{n}{2}-1} \frac{1}{n-k} + \sum_{k=2}^{\frac{n}{2}+1} \frac{1}{n-k} + \frac{1}{n-3}\right)\\
&= \frac{n-6}{n(n-3)} > 0.
\end{aligned}$$

By Lemma 5, $\mathrm{RCW}\left(H_{\lfloor\frac{n-4}{2}\rfloor}\right) < \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right)$ and the result follows if n is odd with $n > 12$ or n is even. □

Theorem 3. *Let $n \geq 7$. If n is odd and $n < 12$, then*

$$\mathrm{RCW}\left(H_{\lfloor\frac{n-4}{2}\rfloor}\right) < \mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right)$$

and $\mathrm{RCW}(G) > \mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right)$ for any n-vertex unicyclic graph G different from $H_{\lfloor\frac{n-4}{2}\rfloor}$ and $G_{\lfloor\frac{n-3}{2}\rfloor}$. Otherwise,

$$\mathrm{RCW}\left(H_{\lfloor\frac{n-4}{2}\rfloor}\right) < \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right)$$

and $\mathrm{RCW}(G) > \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right)$ for any n-vertex unicyclic graph G different from $H_{\lfloor\frac{n-4}{2}\rfloor}$ and $H_{\lfloor\frac{n-6}{2}\rfloor}$.

Proof. Let G be a unicyclic graph with n vertices and diameter d. Then $2 \leq d \leq n-2$. First suppose that $d \leq n-3$. By Lemma 6, we have

$$\mathrm{RCW}(G) \geq f(n,d) \geq f(n,n-3).$$

Case 1. n is odd. If $n < 12$, then

$$\begin{aligned}
f(n,n-3) - \mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right) &= -1 + \sum_{k=3}^{\frac{n+1}{2}} \frac{4}{n-k} + \frac{3}{n-3} - \sum_{k=2}^{\frac{n+1}{2}} \frac{2}{n-k}\\
&= \left(-1 + \sum_{k=3}^{\frac{n+1}{2}} \frac{2}{n-k}\right) + \frac{3}{n-3} - \frac{2}{n-2} > 0.
\end{aligned}$$

If $n > 12$, then

$$\begin{aligned}
f(n,n-3) - \mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right) &= -1 + \sum_{k=3}^{\frac{n+1}{2}} \frac{4}{n-k} + \frac{3}{n-3} - \left(\sum_{k=2}^{\frac{n-3}{2}} \frac{1}{n-k} + \sum_{k=2}^{\frac{n+3}{2}} \frac{1}{n-k} + \frac{1}{n-3}\right)\\
&= \left(-1 + \sum_{k=3}^{\frac{n+1}{2}} \frac{2}{n-k}\right) + \frac{2}{n-3} + \sum_{k=3}^{\frac{n+1}{2}} \frac{2}{n-k} - \sum_{k=2}^{\frac{n-3}{2}} \frac{1}{n-k} - \sum_{k=2}^{\frac{n+3}{2}} \frac{1}{n-k}\\
&> 0 + \frac{2}{n-1} + \frac{2}{n+1} - \frac{2}{n-2} > 0.
\end{aligned}$$

Case 2. n is even. Then

$$f(n,n-3)-\mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right) = -1+\sum_{k=2}^{\frac{n}{2}}\frac{4}{n-k}+\frac{3}{n-3}-\left(\sum_{k=2}^{\frac{n-2}{2}}\frac{1}{n-k}+\sum_{k=2}^{\frac{n+2}{2}}\frac{1}{n-k}+\frac{1}{n-3}\right)$$
$$= \left(-1+\sum_{k=2}^{\frac{n}{2}}\frac{2}{n-k}\right)+\frac{2}{n-3}+\frac{2}{n}-\frac{2}{n-2}>0.$$

Thus, if n is odd and $n<12$ then $\mathrm{RCW}(G)>\mathrm{RCW}\left(G_{\lfloor\frac{n-3}{2}\rfloor}\right)$, otherwise, $\mathrm{RCW}(G)>\mathrm{RCW}\left(H_{\lfloor\frac{n-6}{2}\rfloor}\right)$.

Now suppose that $d=n-2$. Then G is either a graph G_j, where $0\le j\le\lfloor\frac{n-3}{2}\rfloor$, or a graph H_i, where $0\le i\le\lfloor\frac{n-4}{2}\rfloor$. By Lemmas 5 and 7, the result follows. □

By Theorem 3, $H_{\lfloor\frac{n-4}{2}\rfloor}$, $G_{\lfloor\frac{n-3}{2}\rfloor}$ if n is odd and $n<12$, and $H_{\lfloor\frac{n-4}{2}\rfloor}$, $H_{\lfloor\frac{n-6}{2}\rfloor}$ otherwise, are respectively the unique graphs with the smallest, the second smallest RCW numbers in the class of unicyclic graphs with $n\ge 7$ vertices.

4. RCW numbers of bicyclic graphs

Let $L_{n,i}$ be the graph formed from the path P_{n-1} whose vertices are labelled consecutively as $v_0,v_1,\ldots,v_{n-2}$ by adding vertex v and edges vv_i, vv_{i+1} and vv_{i+2}, where $0\le i\le\lfloor\frac{n-4}{2}\rfloor$ (see Fig. 3). It is easily seen that

$$\mathrm{RCW}(L_{n,i})=n-2+\sum_{k=2}^{i+2}\frac{1}{n-k}+\sum_{k=2}^{n-i-2}\frac{1}{n-k}+\frac{1}{n-2}.$$

Theorem 4. *For $n\ge 7$,*

$$\mathrm{RCW}\left(L_{n,\lfloor\frac{n-4}{2}\rfloor}\right)<\mathrm{RCW}\left(L_{n,\lfloor\frac{n-6}{2}\rfloor}\right)$$

and $\mathrm{RCW}(G)>\mathrm{RCW}\left(L_{n,\lfloor\frac{n-6}{2}\rfloor}\right)$ for any n-vertex bicyclic graph G different from $L_{n,\lfloor\frac{n-4}{2}\rfloor}$ and $L_{n,\lfloor\frac{n-6}{2}\rfloor}$.

Proof. Let G be a bicyclic graph with n vertices and diameter d. Then $2\le d\le n-2$. First suppose that $d\le n-3$. By Lemma 6, we have

$$\mathrm{RCW}(G)\ge f(n,d)\ge f(n,n-3).$$

If n is odd, then for $i=\lfloor\frac{n-6}{2}\rfloor$,

$$f(n,n-3)-\mathrm{RCW}(L_{n,i}) = -1+\sum_{k=3}^{\frac{n+1}{2}}\frac{4}{n-k}+\frac{3}{n-3}-\left(\sum_{k=2}^{i+2}\frac{1}{n-k}+\sum_{k=2}^{n-i-2}\frac{1}{n-k}+\frac{1}{n-2}\right)$$
$$=\left(-1+\sum_{k=3}^{\frac{n+1}{2}}\frac{2}{n-k}\right)+\left(\frac{3}{n-3}-\frac{1}{n-2}\right)+\sum_{k=3}^{\frac{n+1}{2}}\frac{2}{n-k}-\sum_{k=2}^{\frac{n-3}{2}}\frac{1}{n-k}-\sum_{k=2}^{\frac{n+3}{2}}\frac{1}{n-k}$$
$$>0+\frac{3}{n-3}-\frac{1}{n-2}+\frac{2}{n+1}+\frac{2}{n-1}-\frac{1}{n-2}-\frac{2}{n-3}-\frac{1}{n-2}$$
$$=\frac{2}{n+1}+\frac{2}{n-1}-\frac{2}{n-2}>0.$$

If n is even, then for $i=\lfloor\frac{n-6}{2}\rfloor$,

$$f(n,n-3)-\mathrm{RCW}(L_{n,i}) = -1+\sum_{k=2}^{\frac{n}{2}}\frac{4}{n-k}+\frac{3}{n-3}-\left(\sum_{k=2}^{i+2}\frac{1}{n-k}+\sum_{k=2}^{n-i-2}\frac{1}{n-k}+\frac{1}{n-2}\right)$$
$$=\left(-1+\sum_{k=2}^{\frac{n}{2}}\frac{2}{n-k}\right)+\left(\frac{3}{n-3}-\frac{1}{n-2}\right)+\sum_{k=2}^{\frac{n}{2}}\frac{2}{n-k}-\sum_{k=2}^{\frac{n}{2}-1}\frac{1}{n-k}-\sum_{k=2}^{\frac{n}{2}+1}\frac{1}{n-k}$$
$$>0+\frac{2}{n-3}+\frac{2}{n}-\frac{2}{n-2}>0.$$

In either case, we have $\mathrm{RCW}(G)>\mathrm{RCW}\left(P_{n,n-2,\lfloor\frac{n-6}{2}\rfloor}\right)$.

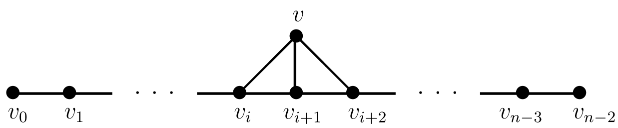

Fig. 3. The graph $L_{n,i}$.

Now suppose that $d = n-2$. Then G is a graph $L_{n,i}$, where $0 \le i \le \lfloor \frac{n-4}{2} \rfloor$. Note that $\mathrm{RCW}(L_{n,i})$ is monotonically decreasing for $0 \le i \le \lfloor \frac{n-4}{2} \rfloor$, and then $\mathrm{RCW}\left(L_{n,\lfloor \frac{n-4}{2} \rfloor}\right) < \mathrm{RCW}\left(L_{n,\lfloor \frac{n-6}{2} \rfloor}\right) < \cdots < \mathrm{RCW}\left(L_{n,0}\right)$. Hence the result follows. $\square$

By Theorem 4, $L_{n,\lfloor \frac{n-4}{2} \rfloor}$ and $L_{n,\lfloor \frac{n-6}{2} \rfloor}$ are, respectively, the unique graphs with the smallest and the second smallest RCW numbers in the class of bicyclic graphs with $n \ge 7$ vertices.

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